

10/513699

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptaeal1624

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	4	APR 07	STN is raising the limits on saved answers
NEWS	5	APR 24	CA/CAPLUS now has more comprehensive patent assignee information
NEWS	6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	7	APR 28	CAS patent authority coverage expanded
NEWS	8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS	10	MAY 08	STN Express, Version 8.4, now available
NEWS	11	MAY 11	STN on the Web enhanced
NEWS	12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS	13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS	14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS	15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS	16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges

10/513699

and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:50:28 ON 22 JUN 2009

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.66

0.66

FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5

DICTIONARY FILE UPDATES: 21 JUN 2009 HIGHEST RN 1159253-26-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

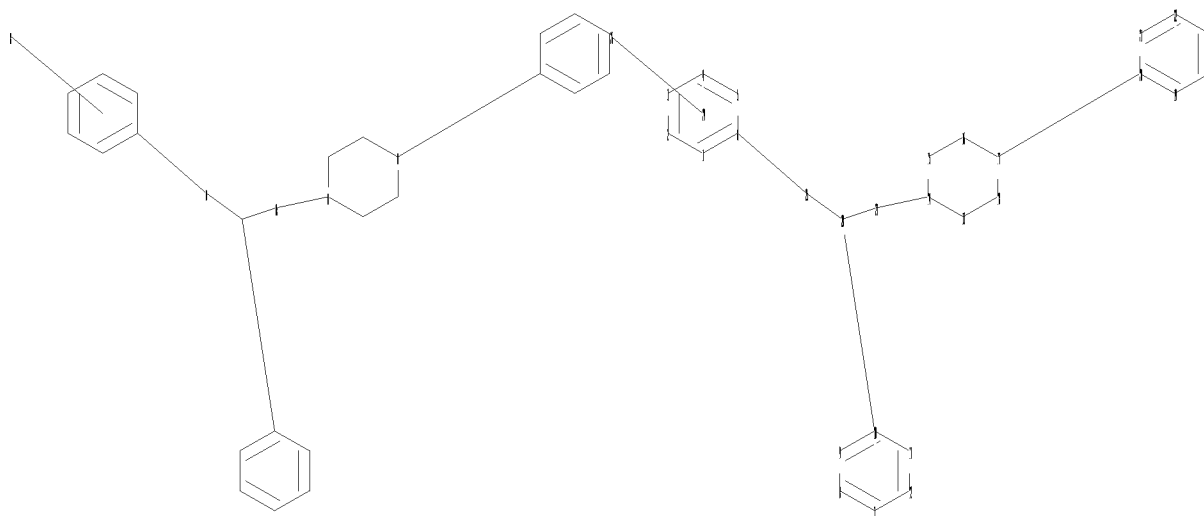
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10594105species.str

10/513699



```
chain nodes :
25 26 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-28 14-27 17-20 25-28 27-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-27 15-16 16-17 17-18 17-20 25-28 27-28
exact bonds :
10-28
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :
```

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:Atom
```

10/513699

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 15:53:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 11045 TO ITERATE

100.0% PROCESSED 11045 ITERATIONS

88 ANSWERS

SEARCH TIME: 00.00.01

L2 88 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.84

187.50

FILE 'CAPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 22 Jun 2009 VOL 150 ISS 26

FILE LAST UPDATED: 21 Jun 2009 (20090621/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

<12/04/2007>

Erich Leese

10/513699

=> s 12 full
L3 2 L2

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 11.28 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

<12/04/2007>

Erich Leese

10/513699

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1103625 CAPLUS

DOCUMENT NUMBER: 143:387060

TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors

INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael

PATENT ASSIGNEE(S): Baylor University, USA

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

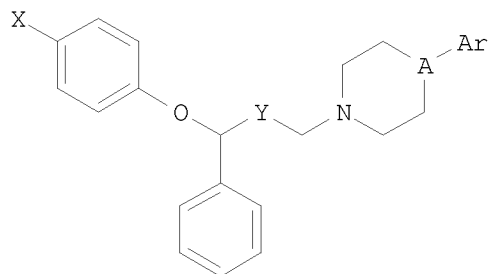
DOCUMENT TYPE: Patent

LANGUAGE: English

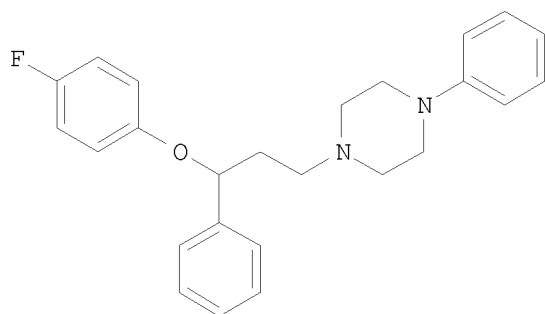
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	-----	-----	-----
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA			
EP 1732610	A2	20061220	EP 2005-730778	20050328
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P	P 20040326
			WO 2005-US10356	W 20050328
OTHER SOURCE(S):	CASREACT 143:387060; MARPAT 143:387060			
GI				



I



II

AB Title compds. I [X = F or CF₃; Y = (CH₂)_n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

IT 691872-56-7P 691872-58-9P 691872-60-3P
691872-62-5P 691872-64-7P 691872-66-9P
866548-21-2P 866548-22-3P 866548-24-5P
866548-25-6P

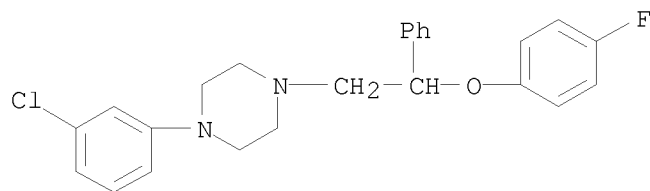
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

RN 691872-56-7 CAPLUS

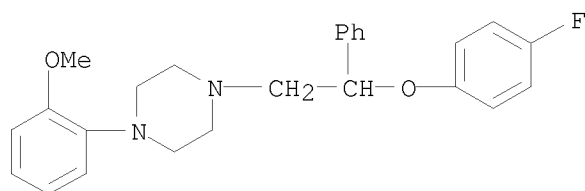
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)

10/513699



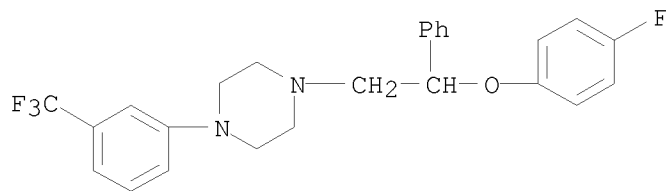
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-
(CA INDEX NAME)



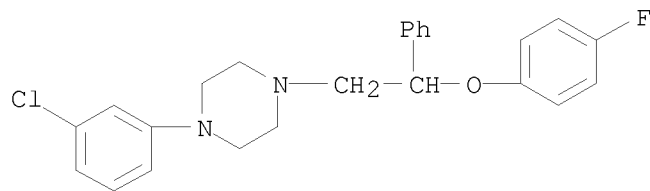
RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-,
hydrochloride (1:1) (CA INDEX NAME)



● HCl

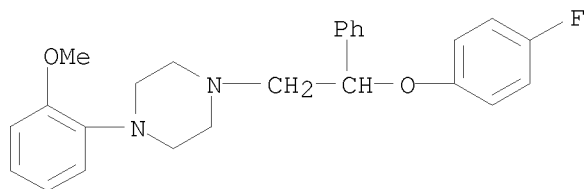
RN 691872-64-7 CAPLUS

<12/04/2007>

Erich Leese

10/513699

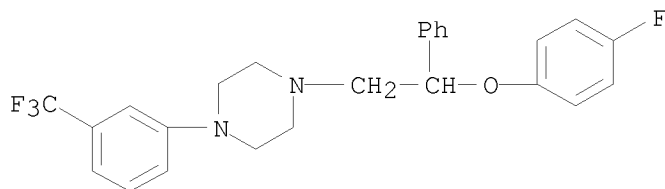
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

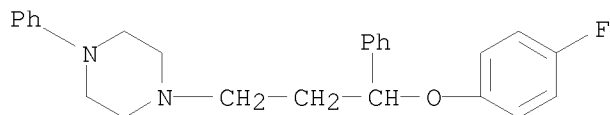
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 866548-21-2 CAPLUS

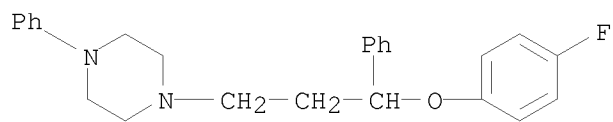
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)



RN 866548-22-3 CAPLUS

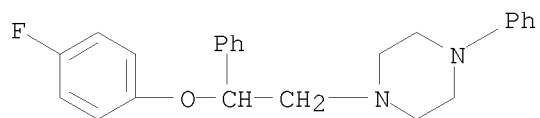
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

10/513699

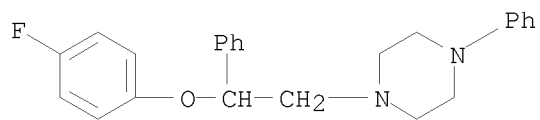


● HCl

RN 866548-24-5 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX NAME)



RN 866548-25-6 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:170822 CAPLUS

DOCUMENT NUMBER: 140:417233

TITLE: Synthesis and biological evaluation of
2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as
serotonin-selective reuptake inhibitors with a
potentially improved adverse reaction profileAUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas
V.; Pinney, Kevin G.CORPORATE SOURCE: Department of Chemistry and Biochemistry and The
Center for Drug Discovery, Baylor University, Waco,
TX, 76798-7348, USASOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6),
1483-1491

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines,
1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine,
1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and
1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-
piperazine, modeled after the potent antidepressant fluoxetine and coupled
with several functionalized piperazines, have been prepared by chemical
synthesis as selective serotonin reuptake inhibitors (SSRIs) with a
potentially improved adverse reaction profile. Typical SSRIs, although
very effective in the treatment of depression, still face the troublesome
side effect of sexual dysfunction. A number of pharmacol. agents-notably,
drugs in the piperazine class-have been used to reverse SSRI-induced
sexual dysfunction, and evidence for developing an improved SSRI by
coupling a fluoxetine congener with the pharmacophore of a reversal agent
holds promise. Preliminary data indicates that the hydrochloride (HCl)
salts of piperazines exhibit single-site binding at the site of the
serotonin reuptake transporter (SERT). However, each of the three compds.
are much less potent than typical SSRIs, showing micromolar (μM)
affinity for the SERT with IC50 values of 1.45 μM , 3.27 μM , and 9.56
 μM , resp. Further biol. evaluation of piperazine compds. is needed
before definitive conclusions can be made with regard to each compound's
potential for use as an SSRI-type candidate which is devoid of sexual side
effects. Nevertheless, the initial findings are quite encouraging, thus
lending credence to the idea of hybridizing an SSRI congener with that of
the pharmacophore of an agent known to reverse or treat SSRI-induced
sexual dysfunction.

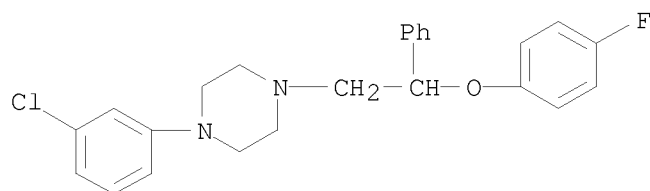
IT 691872-62-5P 691872-64-7P 691872-66-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)(synthesis and structure-activity relationship of
2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake
inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS

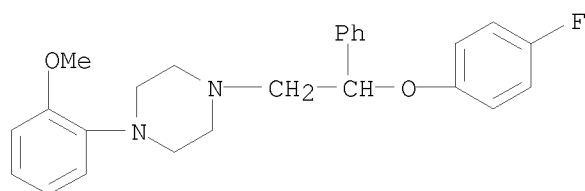
CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-,
hydrochloride (1:1) (CA INDEX NAME)

10/513699



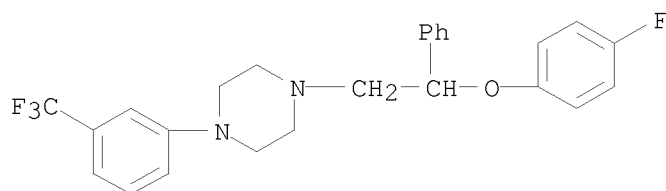
● HCl

RN 691872-64-7 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

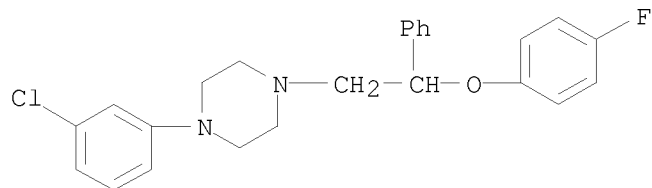
IT 691872-56-7P 691872-58-9P 691872-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and structure-activity relationship of
2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake
inhibitors with a potentially improved adverse reaction profile)
RN 691872-56-7 CAPLUS

<12/04/2007>

Erich Leese

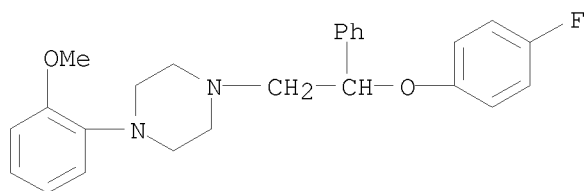
10/513699

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



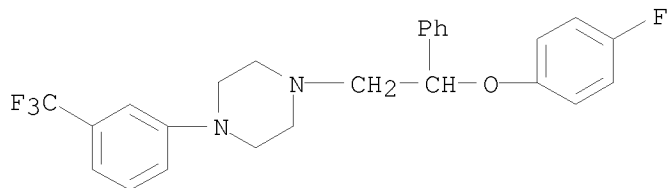
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/513699

=> d his

(FILE 'HOME' ENTERED AT 15:50:28 ON 22 JUN 2009)

FILE 'REGISTRY' ENTERED AT 15:52:03 ON 22 JUN 2009

L1 STRUCTURE UPLOADED

L2 88 S L1 FULL

FILE 'CAPLUS' ENTERED AT 15:53:50 ON 22 JUN 2009

L3 2 S L2 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

20.28

207.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.64

-1.64

STN INTERNATIONAL LOGOFF AT 16:04:47 ON 22 JUN 2009